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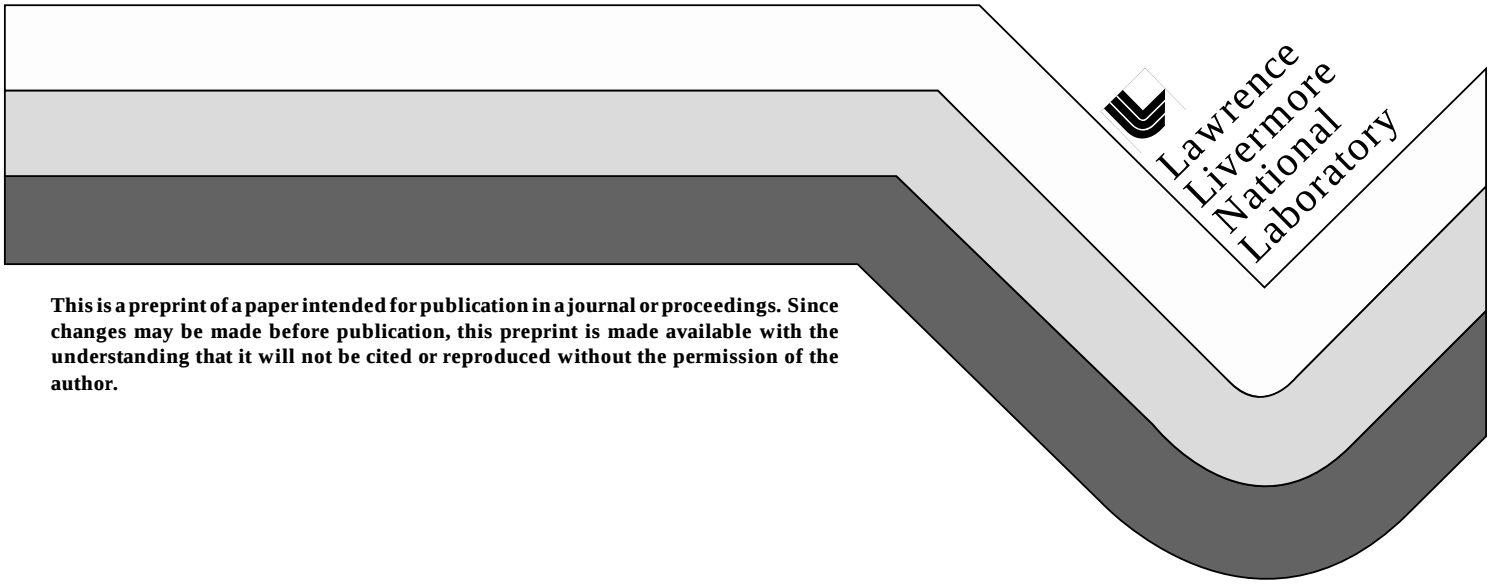

A POINT-CENTERED DIFFUSION DIFFERENCING FOR UNSTRUCTURED MESHES IN 3-D

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ABSTRACT

We describe a point-centered diffusion discretization for 3-D unstructured meshes of polyhedra. The method has several attractive qualities, including second-order accuracy and preservation of linear solutions. A potential drawback to the scheme is that the diffusion matrix is asymmetric, in general. Results of numerical test problems illustrate the behavior of the scheme.

I. INTRODUCTION

Recently there has been increased interest in the design of accurate diffusion differencings for non-orthogonal meshes. Morel and Dendy[1] have developed a cell-centered differencing scheme for 2-D logically-rectangular meshes that is a vast improvement over existing cell-center methods. A point-centered discretization with many of the same properties has been described by Palmer[2]. This scheme has the added benefits of working on an unstructured mesh of polygons and having fewer unknowns than Morel's scheme.

In this paper, we extend the aforementioned point-centered method to three-dimensional unstructured meshes of polyhedra. The method is designed to have the following attractive properties: 1) equivalence with the standard seven-point point-centered scheme on an orthogonal mesh; 2) preservation of the homogeneous linear solution; 3) second-order accuracy; 4) strict conservation within the control volume surrounding each point; and 5) convergence to the exact result as the mesh is refined, regardless of the smoothness of the mesh. A potential disadvantage of the method is that the diffusion matrix is asymmetric, in general.

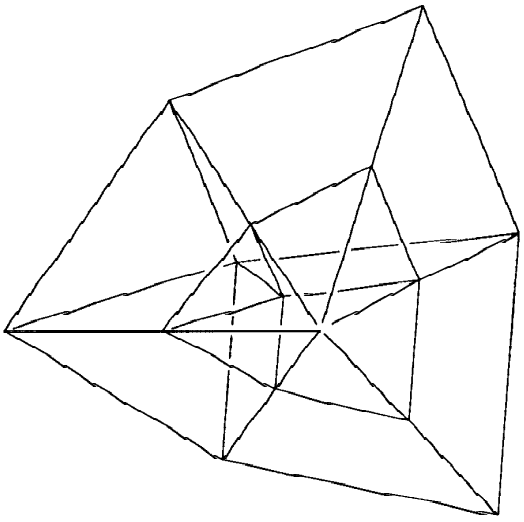

Figure 1: A Portion of an Unstructured Mesh in 3-D.

II. DERIVATION OF THE METHOD

We begin with the time-independent one-group diffusion equation, written as two first-order equations,

$$\overrightarrow{\nabla} \cdot \overrightarrow{J} + \sigma_a \phi = Q, \tag{1}$$

$$\overrightarrow{J} = -D \overrightarrow{\nabla} \phi. \tag{2}$$

Eq. (1) is a statement of balance, i.e. the scalar flux ϕ is conserved. Eq. (2), commonly known as Fick's law, denotes that the current $\overrightarrow{J}$ is proportional to the gradient of the flux ϕ, where the constant of proportionality is the diffusion coefficient D.

We now consider an unstructured mesh of polyhedra in Cartesian geometry, a representative portion of which is shown in Figure 1. Each polyhedral cell is divided into subcell volumes called *wedges*. A wedge is a tetrahedron with vertices at the point p, the zone center z, the face center f and the edge center e. Figure 2 illustrates a wedge (denoted by w) in a cubic zone. The concept of tetrahedral subcell volumes is not our creation. It was originally suggested by Burton[3] in his hydrodynamics work.

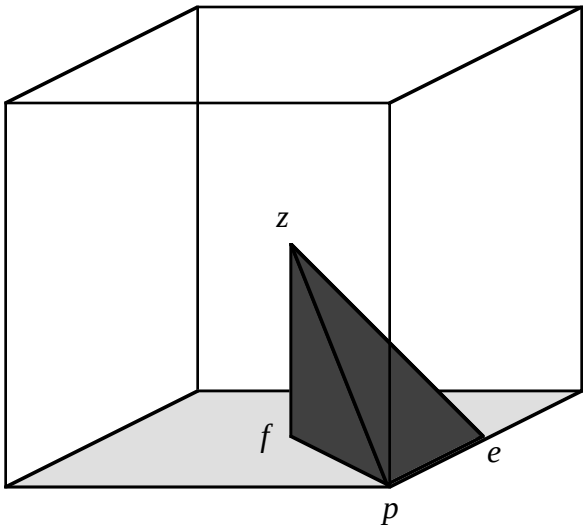

Figure 2: A Wedge in a Cubic Zone.

Our first step is to enforce particle balance by integrating Eq. (1) over the control volume associated with the point of interest. This control volume is defined to be the union of all wedges surrounding the specified point. After performing this integration, we obtain

$$\sum_{w \in p} \overrightarrow{A_{fez,w}} \cdot \overrightarrow{J_{fez,w}} + \left(\sum_{w \in p} V_w \sigma_{a,w} \right) \phi_p = \sum_{w \in p} V_w Q_w, \tag{3}$$

where V_w is the volume of wedge w, ϕ_p is the average flux in the control volume associated with point p, and the term $\overrightarrow{A_{fez,w}} \cdot \overrightarrow{J_{fez,w}}$ should be interpreted as the area of the triangular face fez of the wedge w, times the unit outward normal to that face, dotted into the current $\overrightarrow{J}$ on that face. Our notation $w \in p$ refers to all the wedges w which surround the point p.

The next step in our derivation is the elimination of the currents $\overrightarrow{J_{fez,w}}$. We do this by defining them in terms of fluxes at the points (ϕ_p), zone centers (ϕ_z), face centers (ϕ_f) and edge centers (ϕ_e). Focusing now on the first term in Eq. (3), we can make use of Eq. (2) to write

$$\begin{aligned} \overrightarrow{A_{fez,w}} \cdot \overrightarrow{J_{fez,w}} &= -D_w \left(\overrightarrow{A_{fez}} \cdot \overrightarrow{\nabla} \phi \right) \Big|_w , \\ &= -D_{\tilde{w}} \left(\overrightarrow{A_{fez}} \cdot \overrightarrow{\nabla} \phi \right) \Big|_{\tilde{w}} . \end{aligned} \tag{4}$$

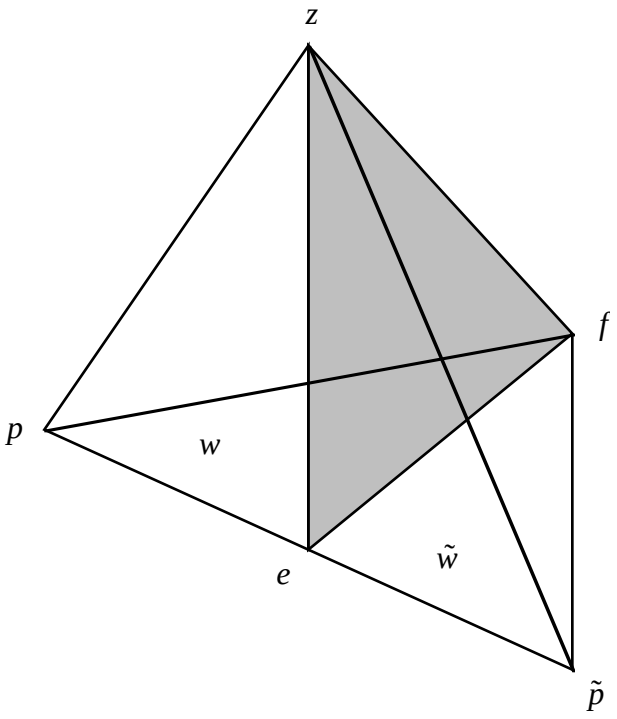

Figure 3: Two wedges: w and $\tilde{w}$.

We have used $\tilde{w}$ to designate the wedge that shares the face fez with wedge w (see Figure 3). Physically, Eq. (4) states that the normal component of the current crossing the face fez is continuous.

The gradient $\overrightarrow{\nabla}\phi$ can be written in terms of the fluxes at the vertices of the wedge if we make use of the following relation:

$$\begin{aligned} \langle \overrightarrow{\nabla}\phi \rangle_w &= \frac{1}{V_w} \int_z d^3r \, \overrightarrow{\nabla}\phi, \\ &= \frac{1}{V_w} \oint_z d^2r \, \overrightarrow{n}\,\phi, \\ &= \frac{1}{V_w} \sum_{f,w} \overrightarrow{A_{f,w}} \phi_{f,w}. \end{aligned} \tag{5}$$

Here, $\overrightarrow{A_{f,w}}$ refers to the area of a face of a wedge, times its unit outward normal.

After a bit of algebra, Eq. (4) becomes

$$\overrightarrow{A_{fez,w}} \cdot \overrightarrow{J_{fez,w}} = \frac{D_w \overrightarrow{A_{fez,w}}}{3V_w} \left(\overrightarrow{A_{fez,w}}\, \phi_p + \overrightarrow{A_{fep,w}}\, \phi_z + \overrightarrow{A_{fzp,w}}\, \phi_e + \overrightarrow{A_{zep,w}}\, \phi_f \right). \quad (6)$$

Our goal is to write Eq. (6) as a function only of point fluxes. We can quickly eliminate the edge flux ϕ_e by imposing the requirement that the normal component of the current crossing the face fez be continuous. We find that the edge flux can be described by

$$\phi_e = (1 - \gamma_w - \delta_w - \delta_{\tilde{w}})\, \phi_f + \gamma_w \phi_z + \delta_w \phi_p + \delta_{\tilde{w}} \phi_{\tilde{p}}, \quad (7)$$

with the associated relations:

$$\gamma_w = -\frac{D_w \left(\overrightarrow{A_{fez,w}} \cdot \overrightarrow{A_{fep,w}} \right) + D_{\tilde{w}} \left(\overrightarrow{A_{fez,\tilde{w}}} \cdot \overrightarrow{A_{fep,\tilde{w}}} \right)}{D_w \left(\overrightarrow{A_{fez,w}} \cdot \overrightarrow{A_{fzp,w}} \right) + D_{\tilde{w}} \left(\overrightarrow{A_{fez,\tilde{w}}} \cdot \overrightarrow{A_{fzp,\tilde{w}}} \right)}, \quad (8)$$

$$\delta_w = -\frac{D_w \left(\overrightarrow{A_{fez,w}} \cdot \overrightarrow{A_{fez,w}} \right)}{D_w \left(\overrightarrow{A_{fez,w}} \cdot \overrightarrow{A_{fzp,w}} \right) + D_{\tilde{w}} \left(\overrightarrow{A_{fez,\tilde{w}}} \cdot \overrightarrow{A_{fzp,\tilde{w}}} \right)}. \quad (9)$$

We note that if $D_w = D_{\tilde{w}}$ the edge flux is a simple average of the two point fluxes ϕ_p and $\phi_{\tilde{p}}$. At this point, our diffusion equation is written in terms of the fluxes at the point, face and zone centers.

Our next task is to define the zone-center fluxes as functions of the point- and face-center fluxes. We choose to define ϕ_z as an inverse-length-weighted average of extrapolations from the point fluxes surrounding that zone; i.e.

$$\phi_z = \sum_{w \in z} w_w \left(\phi_p + \overrightarrow{l_{pz}} \cdot \langle \overrightarrow{\nabla} \phi \rangle_z \right), \quad (10)$$

$$w_w = \frac{\frac{1}{\left| \overrightarrow{l_{pz}} \right|}}{\sum_{p \in z} \frac{1}{\left| \overrightarrow{l_{pz}} \right|}}. \quad (11)$$

These extrapolations involve a zone-averaged gradient $\langle \overrightarrow{\nabla} \phi \rangle_z$, which we define in the same manner as before,

$$\langle \overrightarrow{\nabla} \phi \rangle_z = \frac{1}{V_z} \int_z d^3 r\, \overrightarrow{\nabla} \phi,$$

$$
\begin{aligned}
&= \frac{1}{V_z} \oint_z d^2r \, \overrightarrow{n} \, \phi, \\
&= \frac{1}{V_z} \sum_{f \in z} \overrightarrow{A_f} \phi_f. \qquad (12)
\end{aligned}
$$

where V_z is the volume of the zone, and $\overrightarrow{n}$ is the unit outward normal to the surface of the zone and $\overrightarrow{A_f}$ is the area of the zone face times the unit outward normal to that face. In general this zone-averaged gradient is a function of the fluxes at all the points associated with that zone. We note that the success of our method does not hinge on the choice of inverse-length weighting; other weighting schemes could be used.

The face-center flux is defined in an analogous way,

$$
\phi_f = \sum_{w \in f} v_w \left(\phi_p + \overrightarrow{l_{pf}} \cdot \langle \overrightarrow{\nabla} \phi \rangle_f \right), \qquad (13)
$$

$$
v_w = \frac{\frac{1}{\left| \overrightarrow{l_{wf}} \right|}}{\sum_{w \in f} \frac{1}{\left| \overrightarrow{l_{wf}} \right|}}. \qquad (14)
$$

$$
\begin{aligned}
\langle \overrightarrow{\nabla} \phi \rangle_f &= \frac{1}{A_f} \int_f d^2r \, \overrightarrow{\nabla} \phi, \\
&= \frac{1}{A_f} \oint_f ds \, \overrightarrow{n} \, \phi, \\
&= \frac{1}{A_z} \sum_{w \in f} \overrightarrow{l_{we}} \phi_p. \qquad (15)
\end{aligned}
$$

This completely defines our unstructured diffusion method, aside from boundary conditions. In general, each point is connected to every point associated with the zones surrounding that point. Our definitions for ϕ_z and ϕ_f can cause the diffusion matrix to be asymmetric. As a result, we have chosen to solve the matrix with a biconjugate gradient technique. There are other algorithms that could be used, but we will not concern ourselves with this issue here. On an orthogonal mesh the diffusion operator reduces to the standard point-centered seven-point stencil.

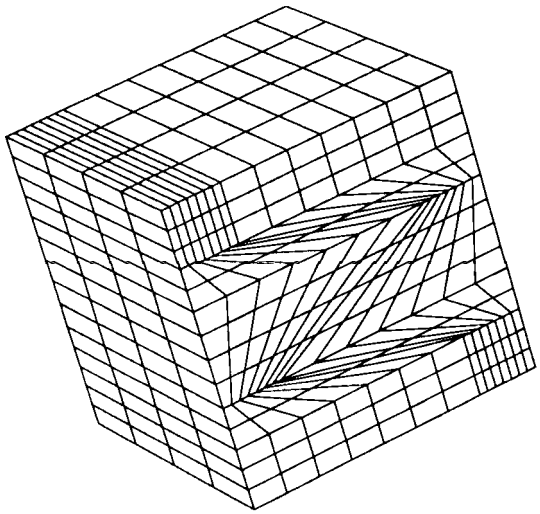

Figure 4: 3D version of Kershaw's "z-mesh".

III. NUMERICAL RESULTS

In this section, we present the results of a few test problems designed to demonstrate that our method preserves the linear solution and is second-order accurate. First we consider a homogeneous, source-free unit cube with reflecting boundaries located at $y = 0$, $y = 1$, $z = 0$ and $z = 1$, a vacuum boundary at $x = 0$, and a unit extrapolated flux $[\phi(1 + 2D, y, z) = 1]$ at $x = 1$. We choose D to be $\frac{1}{1000}$ and set σ_a to 0. We solve this problem on a 3-D version of Kershaw's[4] "z-mesh", as seen in Figure 4. This mesh has 784 $(14 \times 14 \times 4)$ hexahedral zones, some of which have faces that intersect at very acute angles. The exact solution to this problem is linear in the x coordinate,

$$\phi(x, y, z) = \frac{x + 2D}{1 + 4D}. \tag{16}$$

Figure 5 is a contour plot of the solution of this problem in the plane $z = 0.5$. The contours are exactly linear, as they are everywhere in the problem domain. In fact, we obtain the exact solution for this problem, independent of the mesh we are using. This is an important result because other diffusion methods have trouble obtaining the linear solution on these meshes.

A second test problem, suggested by Morel et al[1], is designed to illustrate that the method is second-order accurate and involves the solution of the following diffusion

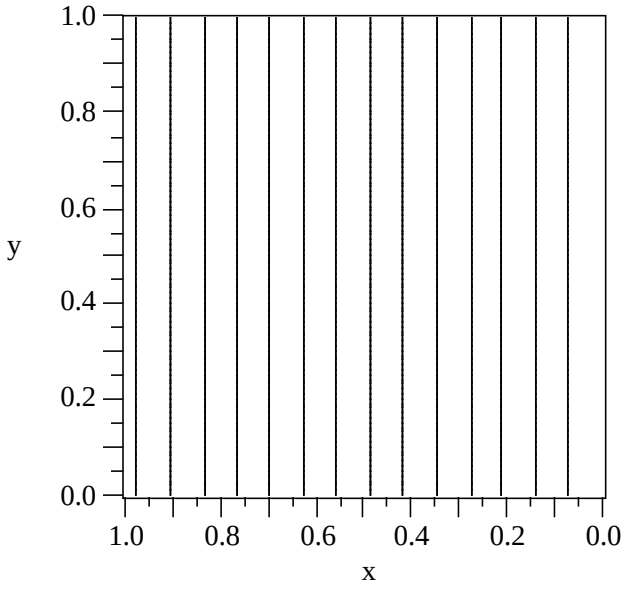

Figure 5: Contours of the solution to the "z-mesh" problem for $z = 0.5$.

problem:

$$-D\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\phi = z^2, \tag{17}$$

with reflecting boundaries located at $x = 0$, $x = 1$, $y = 0$ and $y = 1$, and vacuum boundaries at $z = 0$ and $z = 1$. We choose the diffusion coefficient D to be $\frac{1}{30}$ and set the absorption cross section to zero. The exact solution to this problem is quartic in the z coordinate,

$$\phi(x,y,z) = \frac{1}{12D}\left[\left(\frac{1+8D}{1+4D}\right)(z+2D) - z^4\right]. \tag{18}$$

We solve this problem on five different orthogonal and random meshes of tetrahedra and observe the change in the L_2 norm of the error as a function of mesh size. A typical random mesh is shown in Figure 6. These meshes are constructed in the following manner: 1) a cubic mesh is generated, 2) each cubic zone is divided into 6 tetrahedra, 3) if a random grid is desired, the points are then randomly displaced by some small distance. Figure 7 is a plot of the error as a function of the "mesh size"; that is the grid spacing of the cubic mesh from which the tetrahedral meshes are generated. As we refine the grids, we begin to see that the error goes down by a factor of four as the mesh spacing is halved. The new point-centered method is

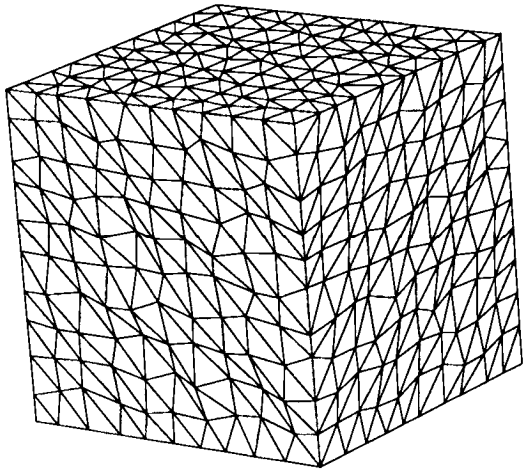

Figure 6: A $10 \times 10 \times 10$ tetrahedral random mesh.

indeed second-order accurate both on the orthogonal and random meshes. This is an important result, for some 2D diffusion discretizations cannot make this claim[4].

IV. CONCLUSIONS

We have successfully extended a point-centered unstructured mesh diffusion scheme to polyhedral grids in 3D Cartesian geometry. The method continues to have many desirable qualities, principally second-order accuracy and preservation of the homogeneous linear solution. It has a potential drawback in that the diffusion matrix is asymmetric in general and must be solved with non-standard iterative techniques. It is worth noting that there are striking similarities between the new method and certain finite-element schemes[5]. However, while they have many of the same characteristics, they are derived using two very different methodologies.

ACKNOWLEDGMENTS

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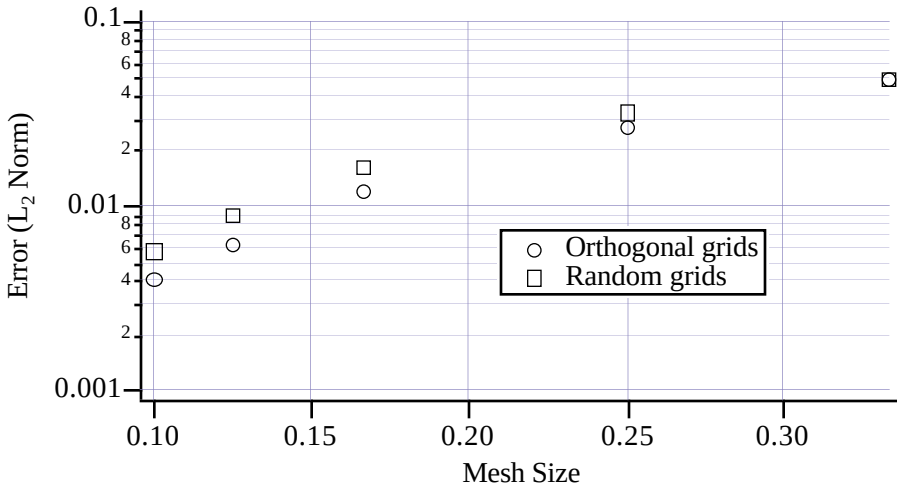

Figure 7: Comparison of errors versus mesh size.

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